

1,3-BUTADIENE

Identified as a toxic air contaminant under California's air toxics program (AB 1807) in 1992.

CAS Registry Number: 106-99-0



Molecular Formula: C_4H_6

1,3-Butadiene is a flammable, colorless gas with a pungent, aromatic, gasoline-like odor. It is insoluble in water, slightly soluble in methanol and ethanol, and soluble in organic solvents such as benzene and ether (U.S. EPA, 1989c). 1,3-Butadiene is a gas at most environmental temperatures and is very volatile even at lower temperatures (HSDB, 1995).

Physical Properties of 1,3-Butadiene

Synonyms: bdivinyl; divinyl; erythrene; vinylethylene; biethylene; pyrrolylene

Molecular Weight:	54.09
Boiling Point:	-4.5 °C at 760 mm Hg
Melting Point:	108.91 °C
Vapor Pressure:	910 mm Hg at 20 °C
Vapor Density:	1.87 (air = 1)
Density/Specific Gravity:	0.6211 at 20/4 °C (water = 1)
Log Octanol/Water Partition Coefficient:	1.99
Conversion Factor:	1 ppm = 2.25 mg/m ³

(HSDB, 1995; Merck, 1989; Sax, 1989; U.S. EPA, 1994a)

SOURCES AND EMISSIONS

A. Sources

In California, the majority of 1,3-butadiene emissions are from incomplete combustion of gasoline and diesel fuels. Mobile sources account for approximately 96 percent of the total annual emissions statewide for quantified sources. Vehicles that are not equipped with functioning exhaust catalysts emit greater amounts of 1,3-butadiene than vehicles with functioning catalysts (ARB, 1992e).

Other sources of 1,3-butadiene include vehicle tire wear, petroleum refining, styrene-

butadiene copolymer production and biomass burning, including residential wood combustion, agricultural burning, and managed forest fires. The largest use of 1,3-butadiene in the United States is in the production of synthetic elastomers, which include: styrene-butadiene copolymer, acrylonitrile-butadiene-styrene resin, polybutadiene, neoprene, and nitrile rubber. Products commonly made from the styrene-butadiene copolymers include tires, mechanical rubber goods, and latex. Latex is commonly used in foam products, paints, carpet and textile backing, paper coatings, and adhesives. The second major national use of 1,3-butadiene is in the production of adiponitrile, the raw material used in nylon 6,6 production (ARB, 1992e).

The primary stationary sources that have reported emissions of 1,3-butadiene are petroleum refining, manufacturing of synthetics and man-made materials, and oil and gas extraction (ARB, 1997b).

B. Emissions

The total emissions of 1,3-butadiene from stationary sources in California are estimated to be at least 22,000 pounds per year, based on data reported under the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b). In 1994, the Air Resources Board (ARB) also estimated that approximately 5.5 million pounds per year were emitted from on-road motor vehicles (ARB, 1995f). The ARB also estimates that emissions from other mobile sources such as off-road recreational vehicles, boats, ships, and trains, contribute an additional 2.6 million pounds of 1,3-butadiene into California's air (ARB, 1995f).

The ARB adopted the Low Emission Vehicles/Clean Fuels regulations in 1990 and the Phase 2 reformulated gasoline regulations in 1991 which is expected to reduce 1,3-butadiene emissions from cars and light-duty trucks (ARB, 1990i; ARB, 1992g).

C. Natural Occurrence

1,3-Butadiene occurs as a product of incomplete combustion in forest fires (HSDB, 1995).

AMBIENT CONCENTRATIONS

1,3-Butadiene is routinely monitored by the statewide ARB air toxics network. When 1,3-butadiene was formally identified as a toxic air contaminant, the ARB estimated a population-weighted annual ambient concentration of 0.82 micrograms per cubic meter ($\mu\text{g}/\text{m}^3$) or 0.37 parts per billion (ppb) (ARB, 1992). The network's mean concentration of 1,3-butadiene from January 1996 through December 1996 is estimated to be $0.466 \mu\text{g}/\text{m}^3$ or 0.207 ppb (ARB, 1997c).

INDOOR SOURCES AND CONCENTRATIONS

Environmental tobacco smoke (ETS) is the primary source of 1,3-butadiene in the indoor environment. Based on measurements of 1,3-butadiene in a tavern, bar, and unventilated lab, the estimated dose of 1,3-butadiene inhaled in three hours in a high tobacco smoke environment could range from 10 to 60 micrograms. In contrast, the estimated dose of 1,3-butadiene inhaled in three hours during exposure to the statewide average outdoor concentration of $0.82 \mu\text{g}/\text{m}^3$ is about 2.6 micrograms (ARB, 1992e).

A recent study sponsored by the ARB measured indoor levels of 1,3-butadiene in 62 Northern California homes during the summer of 1990. Only 5 of the 62 homes had 1,3-butadiene concentrations above the study's limit of detection of $1.2 \mu\text{g}/\text{m}^3$ (0.54 ppb). Results indicate that the concentrations in these five homes ranged from 2.7 to $10.0 \mu\text{g}/\text{m}^3$ (1.22 to 4.53 ppb). In 4 of the 5 homes with measurable 1,3-butadiene, 20 to 40 cigarettes reportedly were smoked during the monitoring period. The source of 1,3-butadiene in the other home with measurable 1,3-butadiene is unknown. Of the homes in this study, smoking occurred in 16 that had concentrations that were less than the detection limit (ARB, 1992e).

Another study sponsored by the ARB determined that the average 1,3-butadiene emission from 6 commercial brands of cigarettes is $152 \mu\text{g}/\text{cigarette}$ (Daisey et al., 1994).

A study conducted in Raleigh, North Carolina found that 1,3-butadiene concentrations within vehicles were about 3 times greater than those measured outdoors. An average 1,3-butadiene concentration of $3.3 \mu\text{g}/\text{m}^3$ (1.5 ppb) and a maximum of $17.2 \mu\text{g}/\text{m}^3$ (7.8 ppb) were measured inside vehicles during commutes (Chan et al., 1991a).

ATMOSPHERIC PERSISTENCE

Dryer and Brezinsky (1986) have shown that 1,3-butadiene is a significant intermediate oxidation product of n-octane, while Venkat, et al. (1992) have shown that butadiene is present as an intermediate in the oxidation of the fuel components benzene, toluene, and ethylbenzene (ARB, 1992).

1,3-Butadiene is removed from the atmosphere by reaction with hydroxyl (OH) radicals, nitrate (NO_3) radicals, and ozone (O_3). The daytime OH radical reaction is calculated to dominate as an atmospheric loss process over the O_3 reaction and over the NO_3 radical reaction. Based on the readily-available data, the initial reaction products from the OH radical, NO_3 radical and O_3 reactions with 1,3-butadiene are acrolein and formaldehyde (plus furan from the OH radical reaction, and organic nitrates from the NO_3 radical reaction) (Atkinson, 1994; Skov et al., 1992). Hydroperoxides are expected from the OH radical reaction in the absence of oxides of nitrogen. Atmospheric half-lives of 1 to 9 hours are expected. Because of its short atmospheric lifetime, 1,3-butadiene is expected to be confined to the local airshed within which it is emitted (Atkinson and Carter, 1984; Atkinson, 1989).

AB 2588 RISK ASSESSMENT INFORMATION

The Office of Environmental Health Hazard Assessment reviews risk assessments submitted under the Air Toxics “Hot Spots” Program (AB 2588). Of the risk assessments reviewed as of April 1996, 1,3-butadiene was the major contributor to the overall cancer risk in 5 of the approximately 550 risk assessments reporting a total cancer risk equal to or greater than 1 in 1 million and contributed to the total cancer risk in 72 of these risk assessments. 1,3-Butadiene also contributed to the total cancer risk in 33 of the approximately 130 risk assessments reporting a total cancer risk equal to or greater than 10 in 1 million (OEHHA, 1996a).

HEALTH EFFECTS

Probable route of human exposure to 1,3-butadiene occurs through inhalation.

Non-Cancer: 1,3-Butadiene vapors are mildly irritating to the eyes and mucous membranes and cause neurological effects such as blurred vision, fatigue, headache, and vertigo at very high levels (U.S. EPA, 1994a). Epidemiological studies of workers in the rubber industry have shown an increase in cardiovascular diseases such as rheumatic and arteriosclerotic heart diseases and blood effects (ATSDR, 1992b). Animal studies have shown respiratory effects, blood effects and hyperplastic changes to the heart from prolonged inhalation exposure to 1,3-butadiene.

The United States Environmental Protection Agency (U.S. EPA) has not established a Reference Concentration (RfC) or an oral Reference Dose (RfD) for 1,3-butadiene (U.S. EPA, 1994a).

No information is available on adverse reproductive or developmental effects of exposure to 1,3-butadiene in humans (U.S. EPA, 1994a). There is evidence of reproductive toxicity in animal studies. 1,3-Butadiene at 6.25 ppm produced ovarian atrophy in female mice. In developmental toxicity studies, 1,3-butadiene has been shown to be fetotoxic in the absence of producing maternal toxicity. At 40 ppm in mice, 1,3-butadiene resulted in reduced fetal weight of males, and at 200 ppm, reduced ossification was reported in fetuses (ARB, 1992e; ATSDR, 1992b).

Cancer: Epidemiological studies of production workers exposed to 1,3-butadiene provide limited evidence of an increased risk of death from hematologic neoplasms, especially leukemia and other lymphomas. Studies of mice exposed to concentrations of 1,3-butadiene indicate that 1,3-butadiene is taken up rapidly by the body and distributed with metabolites to all tissues. This distribution can result in cancer in multiple sites, including the heart, lung, mammary gland, ovaries, forestomach, liver, pancreas, thyroid, testes, and hematopoietic system. Exposure to 1,3-butadiene at higher concentrations is associated with tumors in the rat. It is important to note that 1,3-butadiene is 1 of only 2 chemicals (the other being the fungicide Captafol) known to

induce cancer in the heart of laboratory animals (ARB, 1992e).

The U.S. EPA has classified 1,3-butadiene in Group B2: Probable human carcinogen, with an inhalation potency value of 2.8×10^{-4} (microgram per cubic meter)⁻¹. The U.S. EPA estimates that if an individual were to breathe air containing 1,3-butadiene at $0.004 \mu\text{g}/\text{m}^3$ over a lifetime, that person would theoretically have no more than a 1 in 1 million increased chance of developing cancer (U.S. EPA, 1994a). The International Agency for Research on Cancer has classified 1,3-butadiene in Group 2A: Probable human carcinogen based on limited evidence in humans and sufficient evidence in animals (IARC, 1992). The United States Occupational Safety and Health Administration has proposed that exposure to 1,3-butadiene is associated with an increased risk of death from cancer of the lymphohematopoietic system, and has classified 1,3-butadiene as a potential occupational carcinogen (ARB, 1992e).

The State of California has determined under Proposition 65 and AB 1807 that 1,3-butadiene is a carcinogen (CCR, 1996; ARB, 1992e). The inhalation potency factor that has been used as a basis for regulatory action in California is 1.7×10^{-4} (microgram per cubic meter)⁻¹ (OEHHA, 1994). In other words, the potential excess cancer risk for a person exposed over a lifetime to $1 \mu\text{g}/\text{m}^3$ of 1,3-butadiene is estimated to be no greater than 170 in 1 million. The oral potency factor that has been used as a basis for regulatory action in California is 3.4 (milligram per kilogram per day)⁻¹ (OEHHA, 1994).

